ECE 371
Materials and Devices

09/17/19 - Lecture 8

Kronig-Penney Model and E vs. k

General Information

- Homework #3 assigned, due Tuesday 10/1
- First midterm (covers Ch. 1 and Ch. 2) is on Tuesday 9/24
- Midterm will be closed book/notes and consist of:
  - 5-10 multiple choice questions on Ch. 1 and Ch. 2 material
  - 1 question on crystal planes/lattices
  - 2 questions on quantum mechanics
  - Some relevant equations and constants will be provided
  - Calculators okay
- I will hold a midterm review session and record it. Time and location TBD. Look for an email.
- Previous midterm questions will be posted on the course website on UNM Learn.
- Reading for next time: 3.2

Periodic Potentials

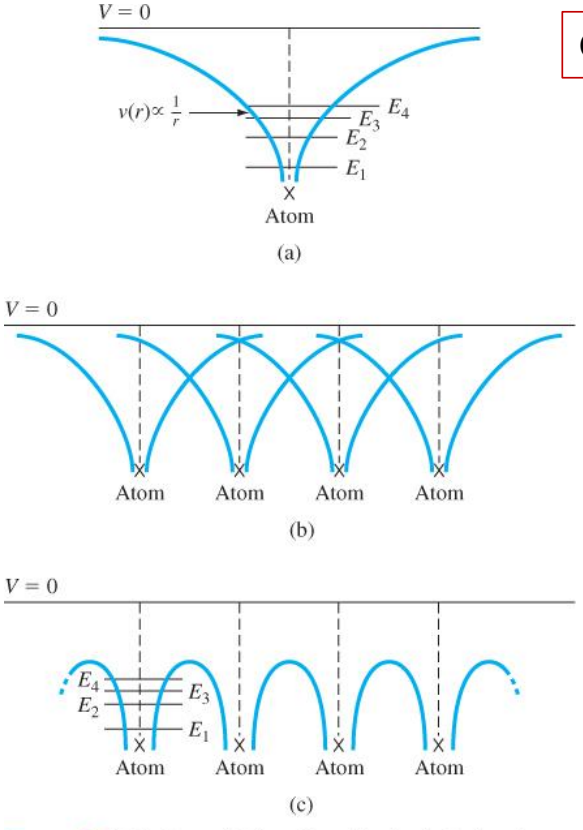


Figure 3.5 | (a) Potential function of a single isolated atom. (b) Overlapping potential functions of adjacent atoms. (c) Net potential function of a one-dimensional single crystal.

Goal: solve Schrodinger equation for a periodic potential

$$V(r) = \frac{1}{4\pi\varepsilon_0}\frac{q_1 q_2}{r}$$

*q is negative for an electron

- When electron and nucleus are far apart, the potential energy is zero
- As they move closer together, it becomes negative (implying we would need to add energy to the system to separate them)
- When atoms interact, the overall potential is lowered
- Real potential shape is difficult to solve analytically

Kronig-Penney Model

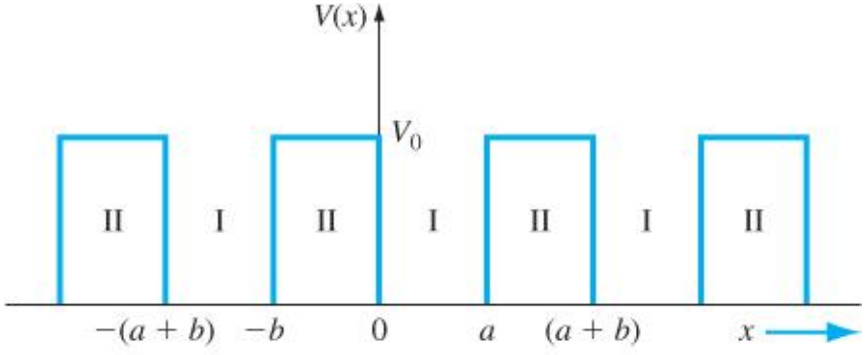


Figure 3.6 | The one-dimensional periodic potential function of the Kronig–Penney model.

- Use 1D array of periodic finite potential wells to model the potential in a crystal
- Solution to Schrodinger equation yields
  - Allowed energy bands
  - Forbidden energy gaps
  - E vs. k relationship (dispersion curve) for electrons
  - Effective mass (m*)
  - Holes (electrons behaving as positive charges)
- Examine the case when $E < V_0$ (electron bound by crystal)

*see in-class derivation

Bloch's Theorem

- Assumption that wave function will not deviate significantly from those of free electrons
- For a periodic potential Bloch showed the wave functions are of the form

$$\psi(x) = u(x)e^{jkx}$$

$u(x)$ is function that is periodic with the crystal lattice and modifies the amplitude

$$u(x) = u\big(x + (a+b)\big) = u\big(x + 2(a+b)\big) = \ \ldots$$

e^{jkx} is the wave function of a free electron

k is the constant of motion or wave number

Kronig-Penney Model

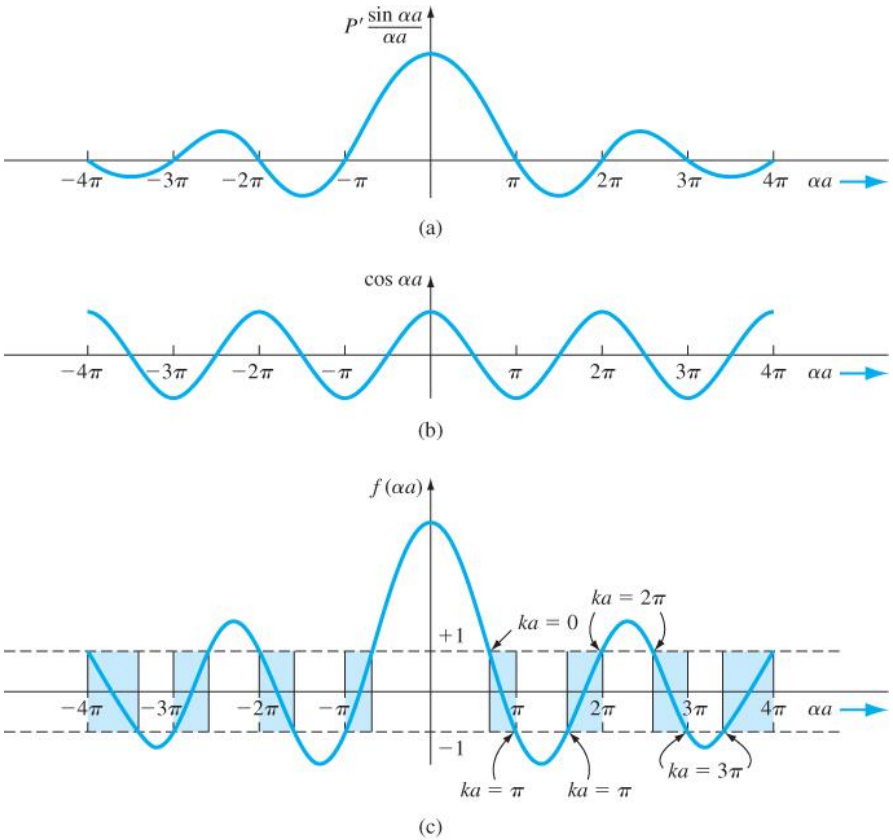


Figure 3.8 | A plot of (a) the first term in Equation (3.29), (b) the second term in Equation (3.29), and (c) the entire $f(\alpha a)$ function. The shaded areas show the allowed values of (αa) corresponding to real values of k.

$$P'\frac{\sin(\alpha a)}{\alpha a} + \cos(\alpha a) = \cos(ka)$$

$$P' = \frac{mV_0 ba}{\hbar^2}$$

- Region where there is a solution to Schrodinger's equation give allowed bands of energies
- If V_0 increases, forbidden bands increase
- As the parameter "a" decreases, the band gap increases

*see in-class derivation

Energy Bands

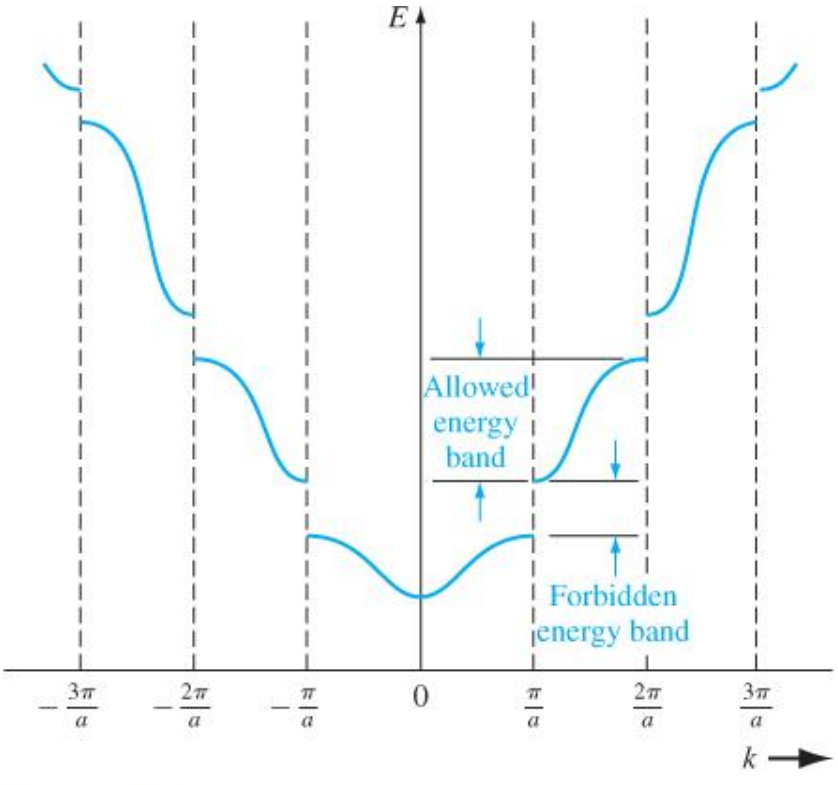
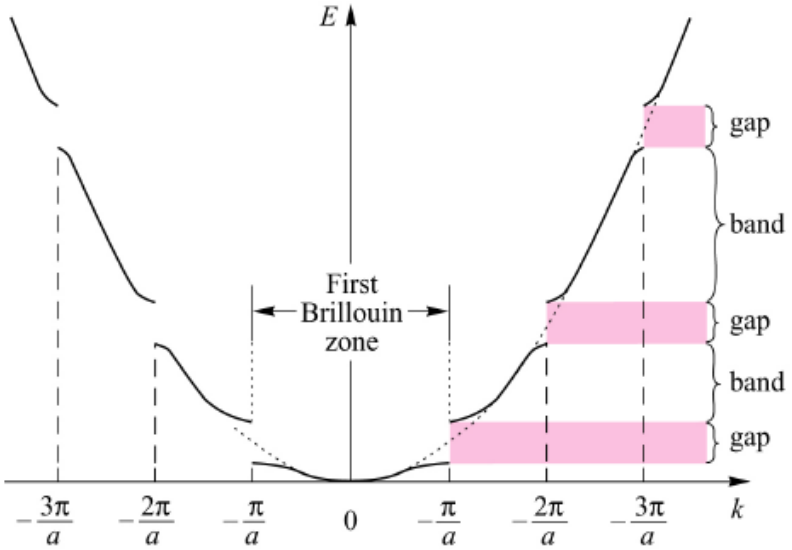


Figure 3.9 | The E versus k diagram generated from Figure 3.8. The allowed energy bands and forbidden energy bandgaps are indicated.

- Kronig-Penney yields concept of allowed and forbidden energies
- Plot E vs. k to reveal the energy bands
- $-\frac{\pi}{a}$ to $\frac{\pi}{a}$ is called the "1st Brillouin zone"

E vs. k - Dispersion Relation

- Significant deviations from the free electron parabolic curve only exist at Brillouin zone boundaries



$$2a = n\lambda$$ Bragg condition!

Energy Band Folding

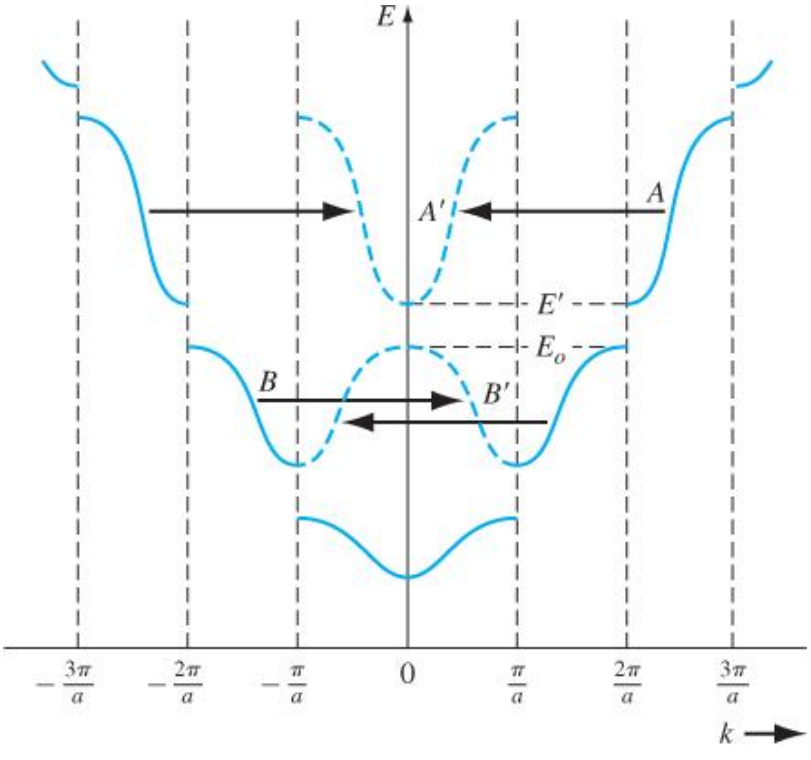


Figure 3.10 | The E versus k diagram showing 2π displacements of several sections of allowed energy bands.

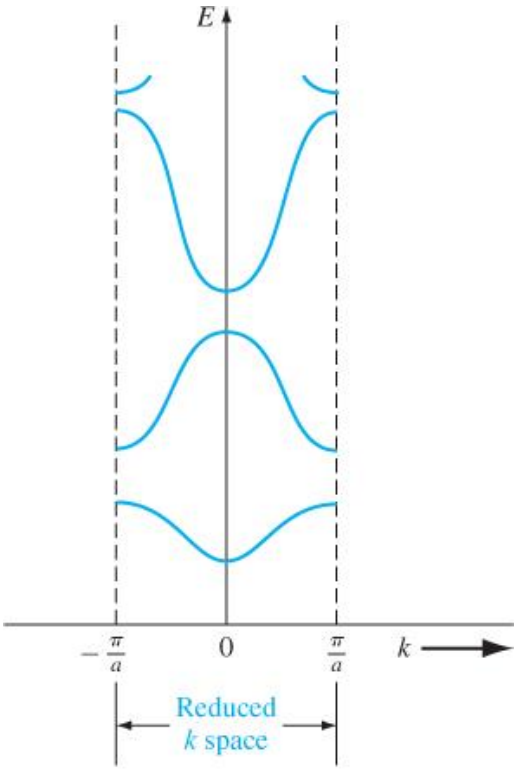


Figure 3.11 | The E versus k diagram in the reduced-zone representation.

E vs. k - Dispersion Relation

- Kronig-Penney model also yields the dispersion relation

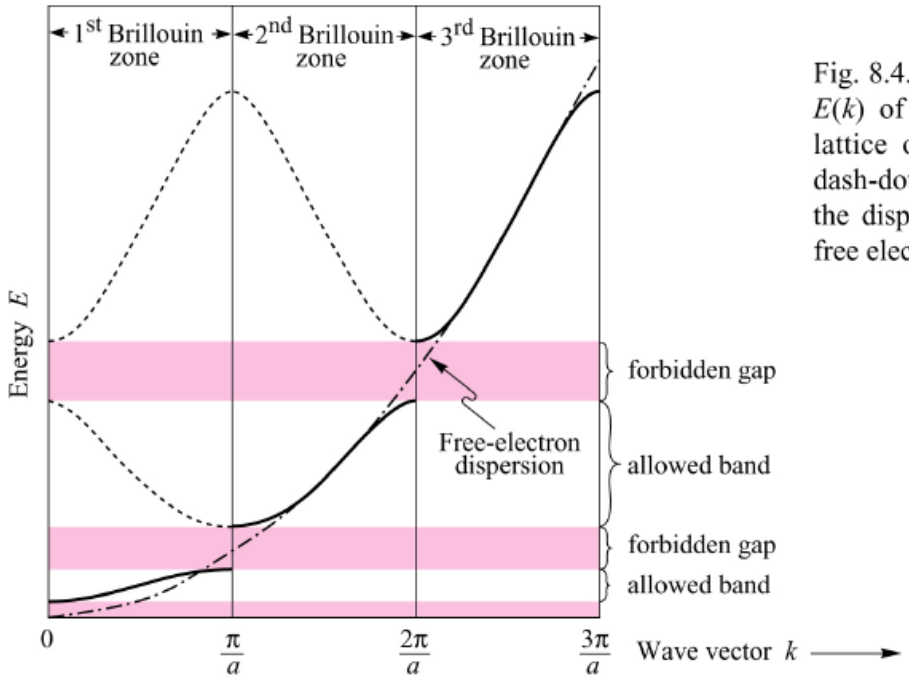


Fig. 8.4. Dispersion relation $E(k)$ of a one-dimensional lattice of a period a. The dash-dotted line represents the dispersion relation of a free electron.

Semiconductor Band Structure

- 3-D: dispersion relation depends on propagation direction since the atomic structure and hence the periodic potential depend on the electron propagation direction

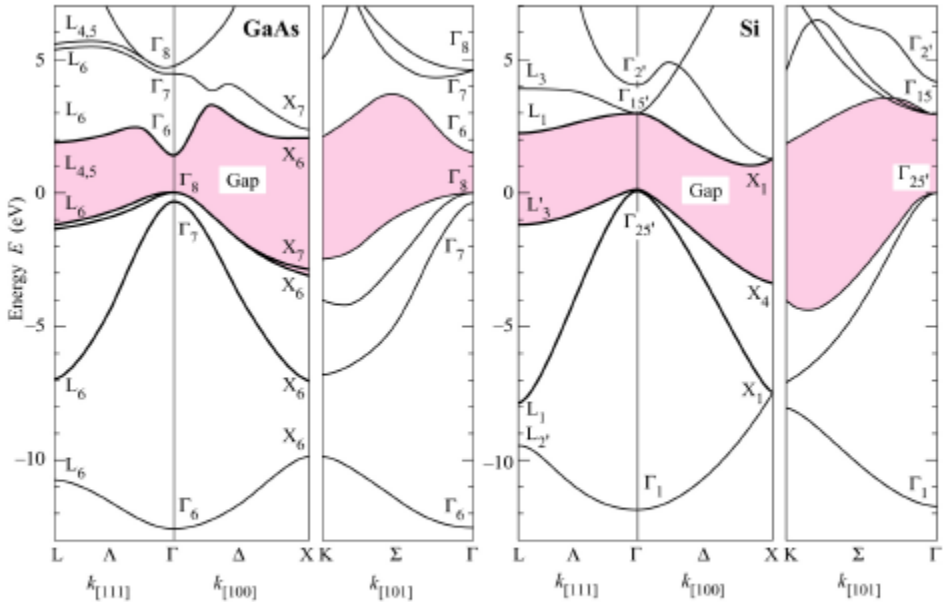


Fig. 8.6 Dispersion relation (band structure) for electrons and holes in the conduction and valence band within the first Brillouin zone for GaAs and Si.

Energy Gap vs. Lattice Constant

- In general, as bond length gets smaller the energy gap increases